

Vibronic spectra of molecules – an experiment with a quantum computer simulator*

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Abstract. In addition to the exciting fundamental questions of quantum computing and implementation possibilities of quantum computers, it is important to look for application areas of quantum computing, to point out practical cases which justify the need for this technology. Besides the well-known qubit-based quantum computers, there are also devices based on other foundations that can surpass the capabilities of classical computers. Among these, devices operating on the basis of boson sampling have a naturally occurring application: the approximate calculation of the vibrational spectrum of molecules. Two separate research groups, Huh et al. [14] and Wang et al. [22] created quantum simulators based on boson sampling, which were successfully used to calculate the transition probabilities between specific states of small molecules. Following the methodology found in these two articles, this paper presents how the calculations of transition probabilities can be performed on a classical computer using a quantum computer simulator which is based on Gaussian boson sampling.

Keywords: Quantum Computing, Gaussian Boson Sampling, Vibronic Spectra of Molecules, Quantum Chemistry, Spectroscopy

AMS Subject Classification: 68Q12, 81P68

*This research was supported by the Ministry of Culture and Innovation and the National Research, Development and Innovation Office within the Quantum Information National Laboratory of Hungary (Grant No. 2022-2.1.1-NL-2022-00004).

1. Introduction

The topic of this paper lies in the intersection of two huge research areas. The first of these is currently one of the hottest, most exciting technology: quantum informatics and quantum computers. Among the countless possible directions, this paper addresses boson sampling, which became the focus of attention after the famous article by Aaronson and Arkhipov [1], in which they proved that the boson sampling problem is difficult to calculate on a classical computer. There are multiple physical implementations of boson sampling, but the most common is the photonic solution, where one-photon states are used as input to an interferometer, and the number of photons is measured at the output. The interferometer is actually the simplest device in the setup; the devices for producing single-photons and for measuring the number of photons are the pinnacle of today's technology, and are constantly being developed. Therefore, it is a much simpler option if we do not use single photons as input, but coherent light, i.e. laser. Since coherent states can be described by Gaussian distributions, this type of boson sampling is called Gaussian boson sampling.

The other major area is – in contrast to quantum informatics – an area that has been actively researched for more than a hundred years, namely spectroscopy, including the examination of the vibrational spectra of molecules. Its importance does not need to be explained, since it has a great influence on our everyday life, for example, on the discovery of novel and more suitable materials for specific scientific, industrial or medical tasks.

There exists an approximate method for determining the vibration spectrum of molecules, in which the probability of transitions between different charged states is calculated. This method can be implemented naturally using Gaussian boson sampling. Our research focuses on this opportunity. Based on Wang et al. [22] and Huh et al. [14], an implementation is presented here which is running on a boson sampling-based simulator, which, in turn, is executed on a classical computer.

The contributions of this paper are (1) an implementation of the algorithm for calculating an approximation of the vibronic spectra of molecules on a photonic quantum computer simulator; (2) the proof that for small molecules this algorithm can be executed on classical computers, which makes testing of photonic quantum computer programs in a simulator possible; and (3) the validation of the results presented in earlier works on the computation of the vibronic spectra of several molecules.

The rest of the paper is structured as follows. Section 2.1 provides a brief introduction to boson sampling and Gaussian boson sampling. Section 2.2 overviews a possible approximate calculation of the vibrational spectra of molecules relying on Gaussian boson sampling. Section 3 presents the implementation of this calculation on a photonic quantum computer simulator. The calculation results are evaluated in Section 4. The achievements of Xanadu, based on the work of Huh et al. [14], are covered in Section 5. Finally, Section 6 sets out future research directions and concludes the paper.

2. Theoretical background

Before elaborating on our experiment with the photonic quantum computer simulator, some basic information of the two aforementioned research areas shall be provided, with a special emphasis on the connection of the two. First the idea of Gaussian boson sampling is introduced, which is one of the main interests of the used simulator, and which gives the algorithmic background for the second component, the approximate computation of the vibronic spectra of molecules.

2.1. Gaussian boson sampling

When talking about quantum computing, discussions tend to begin with the concept of the *qubit*, since it is a widely recognized concept not only among scientists but also among the general public. A qubit is an abstract two-dimensional quantum physical system that can be implemented in various physical forms. It can take on two values (base states), with the Dirac-notation $|0\rangle$ and $|1\rangle$, and can be described using elements of quantum physics, such as a Hilbert space. Qubits can exist in superposition and entangled states with each other. However, these concepts can be extended to larger dimensions, such as the three-dimensional, or any finite-dimensional *qudit*, i.e. $|n\rangle$. Computations are described as unitary operators which act on these states. Moreover, there are two special, non-unitary operators with special purposes: the *annihilation* and *creation operators* (together called as *ladder operators*). These move the physical state from one state to another. For example, if the annihilation operator is denoted as \hat{a} then $\hat{a}|1\rangle = |0\rangle$. The creation operator \hat{a}^\dagger is the adjoint of the annihilation operator. Other important theorems for any finite d -dimensional quantum physical system are the following.

$$\begin{aligned}\hat{a}|n\rangle &= \sqrt{n}|n-1\rangle \\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\ \hat{a}^\dagger\hat{a}|n\rangle &= n|n\rangle \\ \hat{a}|0\rangle &= 0 \quad \text{and} \quad \hat{a}^\dagger|d-1\rangle = 0\end{aligned}\tag{2.1}$$

The product of ladder operators $\hat{N} = \hat{a}^\dagger\hat{a}$ is the number operator. The third equation of (2.1) also shows that quantum states are eigenstates of this number operator in a natural way.

The above can be further generalized to a countably infinite dimension (note that in this case the last equation of (2.1) will make no sense: there will be no state that the creation operator takes to the null vector of the Hilbert space). Bosonic particles are an example of this type of quantum physical system, where unbounded number of particles can be counted in a given state. Such a system is still quantum, i.e. it has superposition and entanglement properties. In the countably infinite dimensional case the quantum physical states are called the *qumodes*.

There is a distribution of states and physical quantities in the case of an arbitrary quantum physical system which can only be determined by multiple mea-

surements, so in fact every quantum computer is a physical implementation of the sampling problem. In the countably infinite-dimensional case this is called boson sampling [10].

Note that the physically feasible operators are all unitary, in the two-dimensional case, for example, the well-known Pauli matrices, the Hadamard gate, or the Controlled Not gate. The physical implementation of boson sampling can be various, but the simplest is still the photonic solution. Quantum optical devices act as unitary operators on the qumode(s). One can find a detailed description of these in quantum optics. The theoretical formula of such devices used in practice with the help of ladder operators is as follows [25].

$$\hat{\mathcal{P}}_i(\phi) = e^{-i\phi\hat{a}_i^\dagger\hat{a}_i} \quad (2.2)$$

$$\hat{\mathcal{D}}_i(\alpha) = e^{\alpha\hat{a}_i^\dagger - \alpha^*\hat{a}_i} \quad (2.3)$$

$$\hat{\mathcal{S}}_i(\zeta) = e^{\frac{1}{2}(\zeta^*\hat{a}_i^2 - \zeta\hat{a}_i^{\dagger 2})} \quad (2.4)$$

$$\hat{\mathcal{B}}_{ij}(\theta) = e^{\theta(\hat{a}_i^\dagger\hat{a}_j - \hat{a}_i\hat{a}_j^\dagger)} \quad (2.5)$$

In order of appearance, the phase shifter, displacement and squeezing operators are acting on one-qumode, and the beam-splitter operator is acting on two-qumodes. These are simple devices from which any linear quantum optical circuit can be assembled. Moreover, any unitary operator can be built using beam-splitters and phase shifters, as an interferometer.

In fact, a pure qumode, i.e. $|n\rangle$ states are technically difficult to produce. The $|1\rangle$ means one photon in a specific qumode. Producing exactly one photon is really a big challenge. For this reason, several easier solutions have been developed to achieve this heavy task [3]. The Gaussian version [12] is particularly important for our research: here, coherent light, viz. a laser, is used as input. A coherent light is nothing more than the sum of countably infinite states for each qumode. For example, if the displacement operator is applied on the vacuum state ($|0\rangle$), the following holds.

$$|\alpha\rangle = e^{-\frac{1}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (2.6)$$

The operators (2.2), (2.3), (2.4) and (2.5) are also called Gaussian operators because they transform coherent states into coherent states. The general coherent state can be achieved starting with a vacuum state and transformed by any product of Gaussian operators above.

The mathematical apparatus for qumodes requires different tools than that of the one-photon states. Since such a system can be described with a Gaussian distribution, the quantum simulator built in this way is called Gaussian boson sampling [24, 25]. Although not used here, note that this can be further extended to continuous-variable systems. More information on Gaussian states and this topic can be found in many articles [11, 18].

2.2. Vibronic spectra of molecules

Besides the brief description of the vibration spectrum of molecules given here, more detailed descriptions can be found in Huh's thesis [13] and many other sources [15, 21, 27]. One of the main issues of spectroscopy is the examination of the electrical transitions of atoms and molecules, whether they take place between states of the same or different electrical charges. However, with the exception of the hydrogen atom, which can be solved exactly, the quantum mechanical equations become exponentially more complex with the number of electrons, and their calculation becomes expensive or practically impossible. Therefore, approximate methods must be found; here, for instance, the path leading to the method of calculating coherent states with the help of operators acting on them is presented.

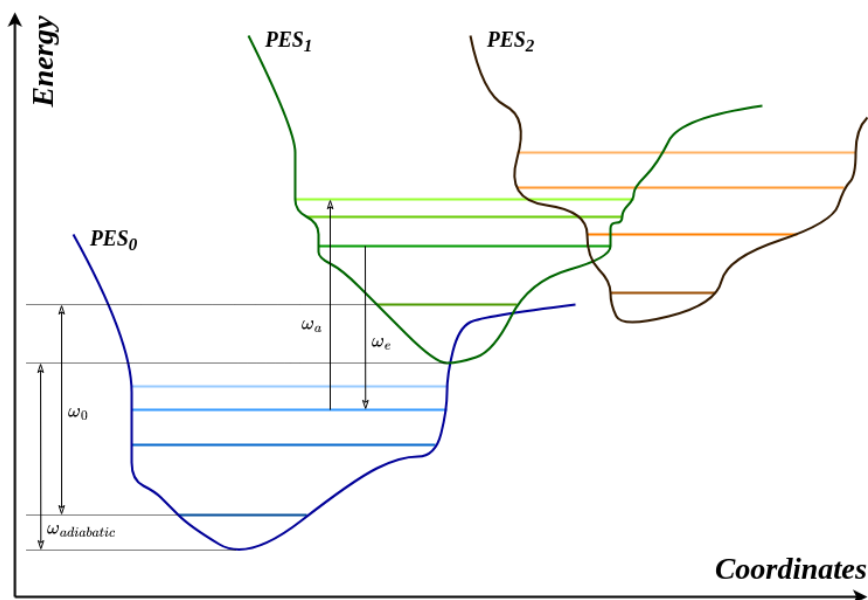


Figure 1. Transitions between molecular states. The curves represent different electronic *potential energy surfaces* (*PES*). Transitions are possible between any two *PES*, however the picture takes into account only the transitions for our interest, i.e. the states of q molecule with different electronic charges. Here ω_a is the angular frequency of one-photon absorption, while ω_e stands for the angular frequency of one-photon emission.

A good approximation of enormously complex system of molecules, if the nuclear and electron states are assumed to be independent, is called the Born-Oppenheimer approximation [2]. Also, due to their mass, atomic nuclei react more slowly to changes in the electron shell, so the nuclei can be considered as a constant background in Franck-Condon principle [6, 9].

With approximating the vibration of electrons with simple quantum harmonic oscillators, one can write the Hamiltonian operator of electrons as a function of the reaction coordinates. Then the potential electron surface can already be described by a parabola.

$$\hat{\mathcal{H}} = \hat{\mathbf{p}}^2 + \hat{\mathbf{q}}^2 \quad (2.7)$$

Here $\hat{\mathbf{q}}$ are the mass-weighted normal coordinates and $\hat{\mathbf{p}}$ are the canonical moments. Duschinsky [7] used another approximation, assuming a linear relationship between the normal coordinates of the different electronic states.

$$\hat{\mathbf{q}}' = \mathcal{U}_{Dusch} \hat{\mathbf{q}} + \hat{\mathbf{d}} \quad (2.8)$$

This introduces the real \mathcal{U}_{Dusch} mixing matrix, as well as the real $\hat{\mathbf{d}}$ displacement operator.

Doktorov and et al. [8] showed that under these conditions, for the states of such linearly connected quantum harmonic oscillators the relation between quantum states $|\phi\rangle$ and $|\phi'\rangle$ of different *PES* can be given in the following way.

$$|\phi'\rangle = U_{Dokt} |\phi\rangle \quad (2.9)$$

Here the so-called Doktorov-operator is defined as follows.

$$\hat{U}_{Dok} = \hat{D}(\hat{\mathbf{d}}) \hat{S}^\dagger(\Omega') \hat{R}(U_{Dusch}) \hat{S}(\Omega) \quad (2.10)$$

That is, the Doktorov operator can be written as a product of unitary Gaussian operators, with the help of one-mode squeezings \hat{S} , the rotation \hat{R} and the displacement operator \hat{D} . The input parameter of the rotation operator is the Duschinsky mixing matrix itself, and the argument of the displacement operator \hat{D} is the Duschinsky displacement from equation (2.8).¹ The squeezings are derived from the physical characteristics of the molecule, specifically Ω and Ω' are the harmonic angular frequencies of the atoms within the molecule in pre- and post-transition states.

The solution of the (2.7) eigenvalue problem is the coherent states in Fock-space. The peculiarity of the Gaussian operators acting on them is that they transform a coherent state to a coherent state.

The transition probabilities – the so-called Franck-Condon factors – between the different electronic states can be approximated using the previous definitions as follows.

$$FCF_{\mathbf{n}', \mathbf{n}} = |\langle \phi' | \phi \rangle|^2 = |\langle \mathbf{n}' | U_{Dokt} | \mathbf{n} \rangle|^2 \quad (2.11)$$

The power of boson sampling is the implementation of a rotation matrix acting on qumodes. In our case of calculating the vibronic spectra, the Doktorov operator (2.10) is used, containing the $\hat{R}(U_{Dusch})$ rotation operator. Thus, the transition probabilities (2.11) can be obtained by passing a properly prepared coherent state through a boson sampling device, and after applying another squeezing, the modes and thus the factors can be measured.

¹Note that the Duschinsky displacement added to the normal coordinates and the Gaussian displacement acting on the quantum states are different concepts.

3. Implementation of the experiment

For a Gaussian boson sampling task, building a quantum computer operating on such a principle is of course the most adequate approach. Although this is no longer an impossible task, it is still difficult and expensive. Huh et al. [14] and Wang et al. [22] implemented these measurements in hardware. The former group used a photonic solution, where the rotation operation was provided by an interferometer, but in a modified form, since the photons coming out of the interferometer could be measured directly by the photon number detectors. The other group implemented the calculation of (2.11) with trapped ions (also Shen et al. [20] created such a device), so they could directly implement the resolution of the Doktorov transformation by (2.10) Gaussian operators.

Another possible, albeit limited solution is to create a simulator based on boson sampling which can be executed on a classic computer. In this experiment Piquasso [5], an open-source photonic quantum computer simulator was used. Piquasso provides a domain-specific programming language to describe quantum optical circuits. This language is embedded into Python, and the simulator front-end is also implemented in Python. The back-end of the simulator can either be executed in Python, or, in the case of Piquasso Boost, in C++.

```
with pq.Program() as program:
    for i in range(modes):
        pq.Q(i) | pq.Squeezing(r = pre_transition_squeezing[i])
    pq.Q() | pq.Interferometer(U_duschinsky)
    for i in range(modes):
        pq.Q(i) | pq.Squeezing(r = (-1) * post_transition_squeezing[i])
    for i in range(modes):
        pq.Q(i) | pq.Displacement(a = displacement[i])
    pq.Q() | pq.ParticleNumberMeasurement()

config = pq.Config(cutoff = cutoff, measurement_cutoff = measurement_cutoff)
simulator = pq.GaussianSimulator(d = modes, config = config)
result = simulator.execute(program, shots = shots).samples
```

Figure 2. Code snippet about circuit of Gaussian boson sampling calculating vibronic spectra of molecules.

In Figure 2 the photonic quantum computer code for calculating vibronic spectra can be seen in Piquasso. Here *pq* is the abbreviation of the Piquasso package, and the operators provided by the package are easy and clear to interpret and use. With the help of Piquasso, the circuit seems quite simple, but of course behind the application of every Gaussian operator there is a multiplication of matrices with exponentialized matrices, as one expects due to (2.2), (2.3), (2.4) and (2.5). Because of the infinity power series of exponential, we need to introduce finite cut-offs. The dimensionless arguments of the operators are derived from the physical parameters of the given molecule. To determine the distribution more precisely, several measurements are required, typically a few thousand runs.

The calculation of Franck-Condon factors (2.11) at temperature 0 K, i.e. $|\mathbf{n}\rangle = |0\rangle$ is calculated on the pre-transition base state. This can be expanded to any

$|n\rangle$ also for pre-transition modes, using a new one-mode squeezing operator at the beginning of the calculations, see [19, Equation 51].

4. Result

Now the calculations of transitions of three molecules, namely the formic acid (Figure 3), ozone (Figure 4) and nitrogen dioxide (Figure 5) are presented. The calculation of the Franck-Condon factors of the first molecule on a boson sampling-based quantum simulator was performed by Huh et al. [14]. The calculation of the Franck-Condon factors of the other two molecules was carried out by Wang et al. [22], and in their case, simulation was also measured with single-bit extraction. Furthermore, their article contains the values of transition probabilities calculated classically and with master equation as well. These data can be found in the Supplemental Material of their article on arXiv [23]. The physical parameters of the molecules can be found in the above articles, and also in the Nist database [17].

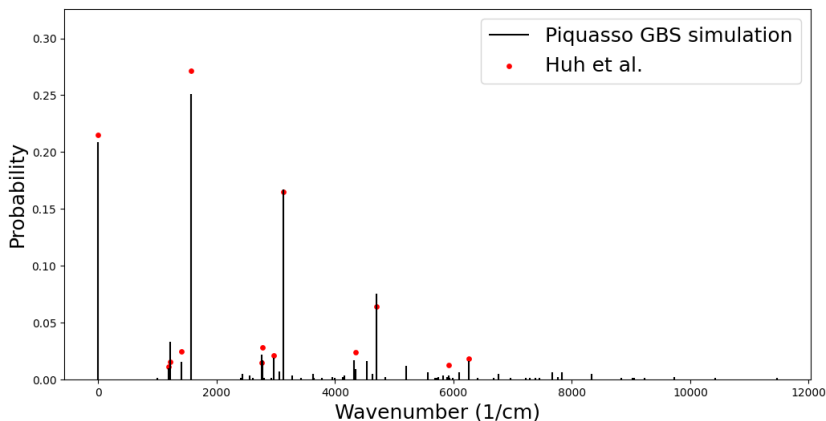


Figure 3. Formic acid $1^1A'$ ($n = 0, m = 0$) \rightarrow $1^2A''$ transition.

The calculation time of transition probabilities with the Piquasso [5] boson sampling-based simulator increases drastically (exponentially) with the increase of the cutoff value. In the case of formic acid, it is sufficient to set the cutoff value for the number of qumodes, but for the other two molecules it is worthwhile to choose the total number of photons that can be measured on the output (two qumodes), as found in the Supplemental Material [23].

In the case of ozone and nitrogen dioxide, which have C_{2v} point group symmetry, a negative anion emits an electron, and the molecule becomes neutral. The formic acid molecule has C_s point group symmetry.

For the convergence of the sampling process, the formic acid case required 1 000 runs of the quantum program, but the other two molecules needed 10 000 runs. The

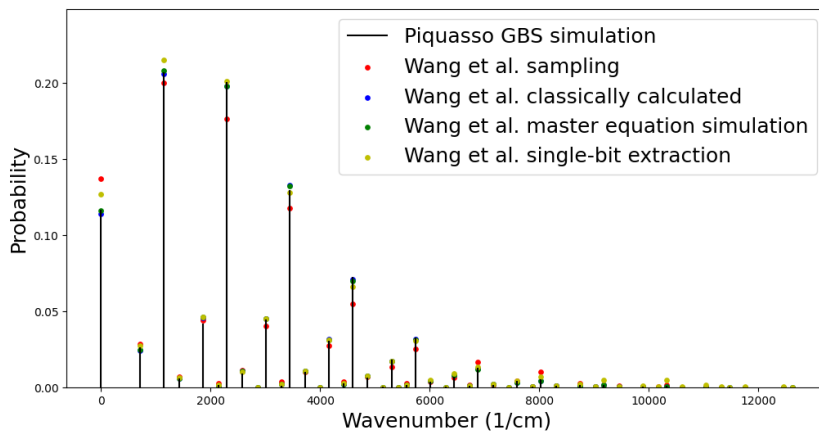


Figure 4. Spectrum of $O_3^-(n=0, m=0) \rightarrow O_3 + e^-$ transition.

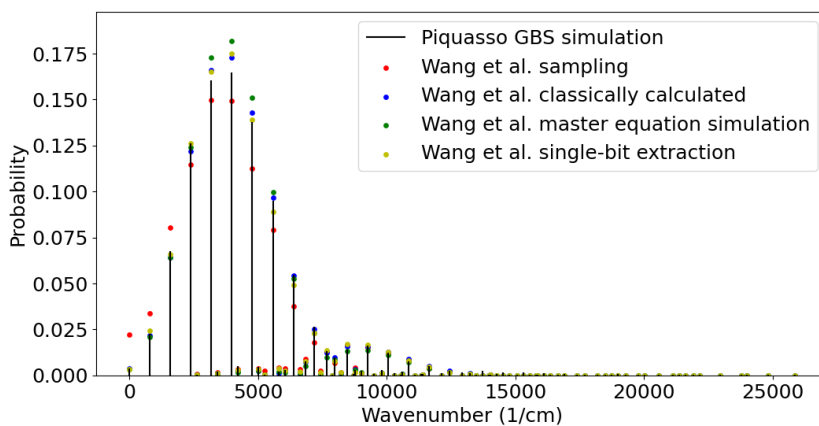


Figure 5. Spectrum of $NO_2^-(n=0, m=0) \rightarrow NO_2 + e^-$ transition.

computations were performed with the Piquasso Python back-end on a standard PC (i7 1.9 GHz with 16 GB memory), and required less than 1 hour.

5. Related work

The Strawberryfields application of Xanadu [26] is another boson sampling based quantum simulator, also written in the Python programming language. This software is a stepping stone for available photonic quantum computers developed by Xanadu. Such a quantum hardware environment does not yet exist behind Piquasso, therefore the latter relies on the resources of classical computers. More in-

formation about the Xanadu Strawberryfields simulator can be found in the works of Bromley et al. [4] and Killoran et al. [16].

Similar to the Piquasso simulator, a circuit simulating the vibration spectrum of molecules can also be implemented in Xanadu's simulator. The physical data of formic acid, water and pyrrole molecules can also be found in Strawberryfields, with which the Franck-Condon factors of these molecules can be easily calculated. The simulation results for the formic acid in Piquasso and Strawberryfields perfectly match, but the Piquasso-based implementation is faster, especially with the Piquasso Boost back-end. The difference in execution time was significant for the experiments with 10 000 runs.

6. Conclusion

The circuit developed in the Piquasso photonic quantum computer simulator successfully calculated the Franck-Condon factors of the vibrational spectra of three molecules: formic acid, ozone and nitrogen dioxid, yielding similar results to those found in Huh et al. [14] and Wang et al. [22]. The simulator executed the Gaussian boson sampling algorithm on a classical computer. Although computations for larger molecules would exceed the resources of classical computers, our results show that smaller molecules can be handled with this technology. This makes it possible to experiment with affordable devices in order to further improve the algorithm and possibly the quantum chemical model. Another important consequence of the presented experiment is that programs written for quantum computing devices can be effectively tested in a simulator, hence facilitating the development of such applications.

It is important to note that the disadvantage of a simulator based on Gaussian boson sampling compared to a physically realized quantum computer built on a similar principle is its finite calculation capacity, i.e. the application of a cutoff is necessary to limit the maximum value of the qumodes in the case of the former, while the latter is only hindered by the limitations of the detectors.

There are many open research possibilities in the topic: testing the existing algorithm, extending it to calculate new transitions of existing molecules, but also to extending it to additional molecules. Furthermore, the limits of the simulators that can be run on classical computers can be measured, either depending on the number or the maximum value of the qumodes. In the more distant future, an automated search for suitable molecules with transitions optimized for a given task is conceivable.

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